Shear Viscosity of Molten Potassium Chloride from Equilibrium and Nonequilibrium Molecular Dynamics Simulations

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During the past 30 years there have been many simulations of the properties of molten alkali halides although relatively few results have been presented for the thermal transport properties other than self-diffusion. These thermal transport properties are difficult to measure experimentally, yet are of great interest--especially in the design of high temperature fuel cells. In this work equilibrium (EMD) and nonequilibrium molecular dynamics (NEMD) simulations have been used to calculate the shear viscosity of these materials. In particular, the simulations were performed for potassium chloride in the canonical ensemble using the Born-Mayer-Huggins-Tosi-Fumi interionic potential model. The NEMD simulations have been performed using the Gaussian isokinetic SLLOD algorithm and are compared with the results obtained through EMD simulations with the Green-Kubo method. The Coulombic interactions have been calculated through the Ewald sum method. Analysis of the system-size dependence is performed for both of the simulation methods. The results are in satisfactory agreement with each other and with available experimental data.